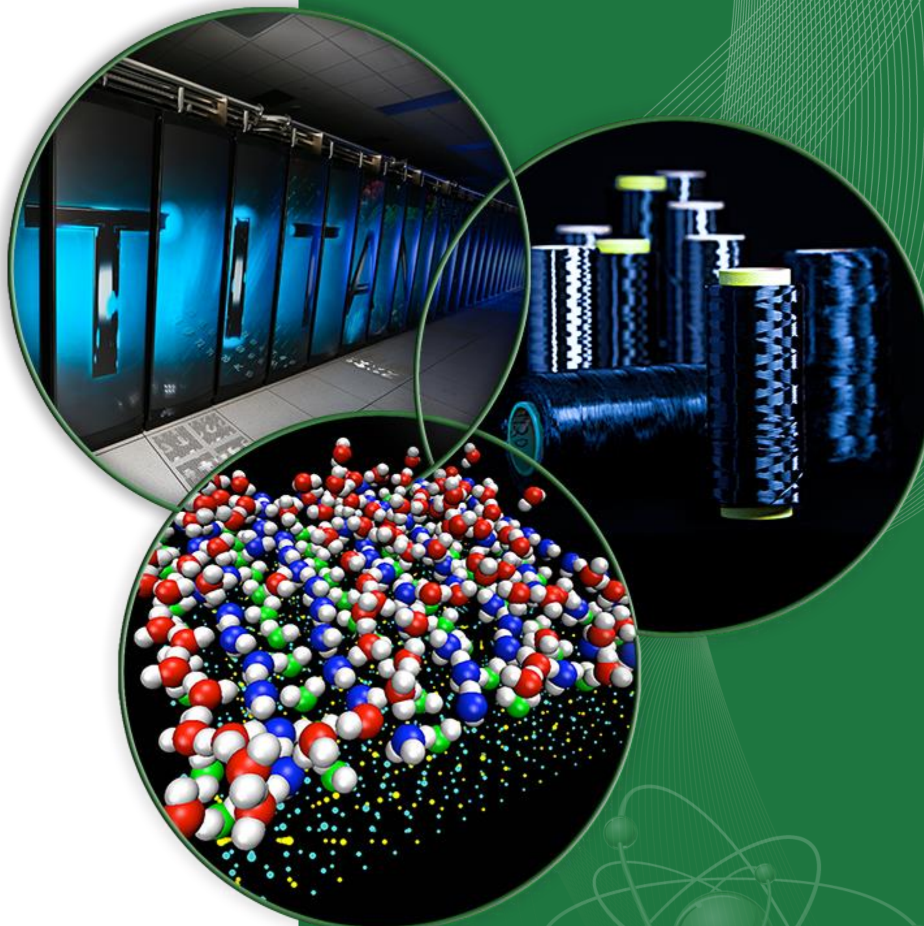
Effective interactions and operators from coupled-cluster theory



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ICNT: Theory for open-shell nuclei near the limits of stability

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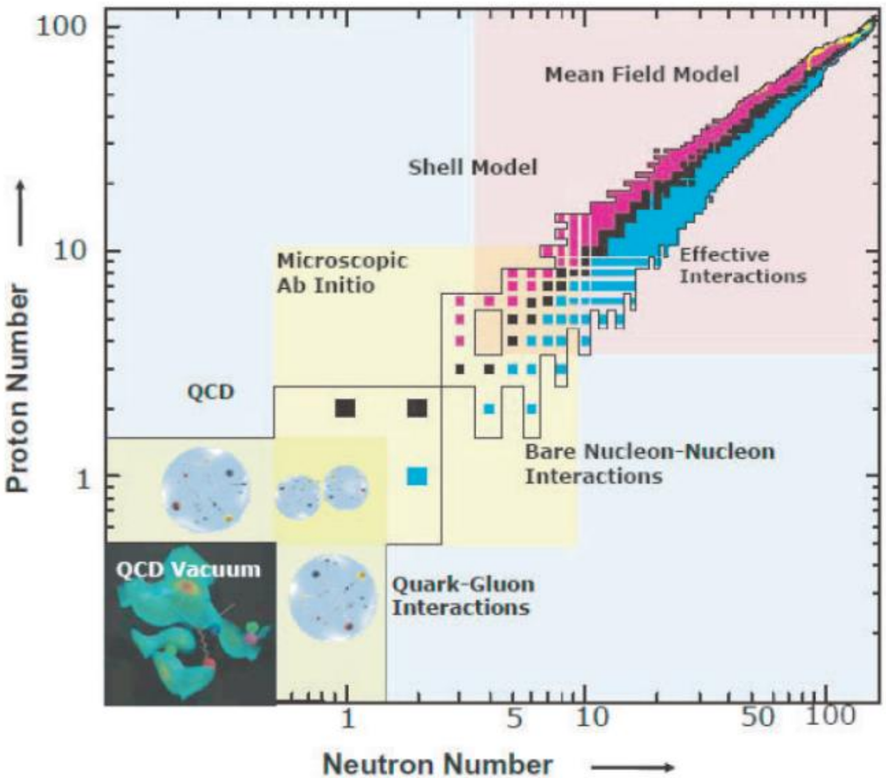
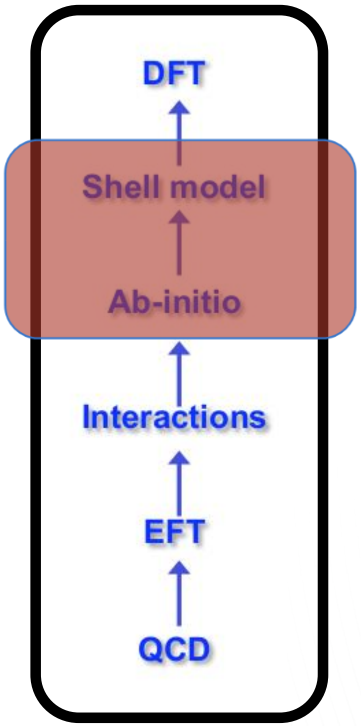
Outline

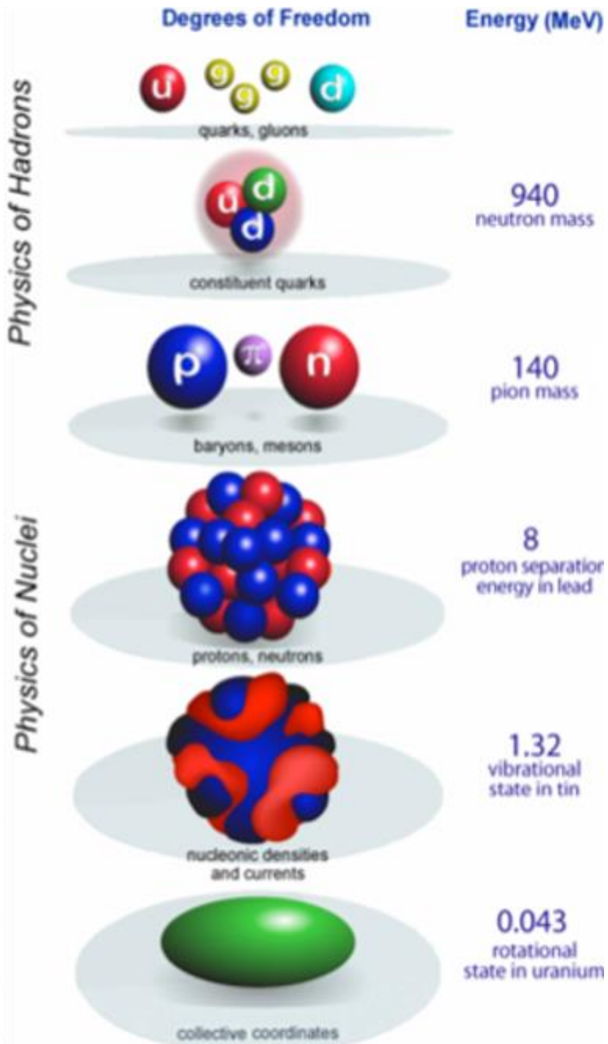
- Motivation
- Coupled-cluster theory
- Coupled-cluster effective interaction (CCEI)
- Results
- Work in progress
- Outlook

Overview

- *Arrive at a Hamiltonian (a "standard model") of nuclear physics*
- *Understand the link between (Lattice) QCD and EFT and nuclei*
- *What are the limits for the existence of nuclei (i.e. drip line location)*
- *Explain collective phenomena from individual motion of nuclei*
- *Error estimates of computed quantities*
- *….*





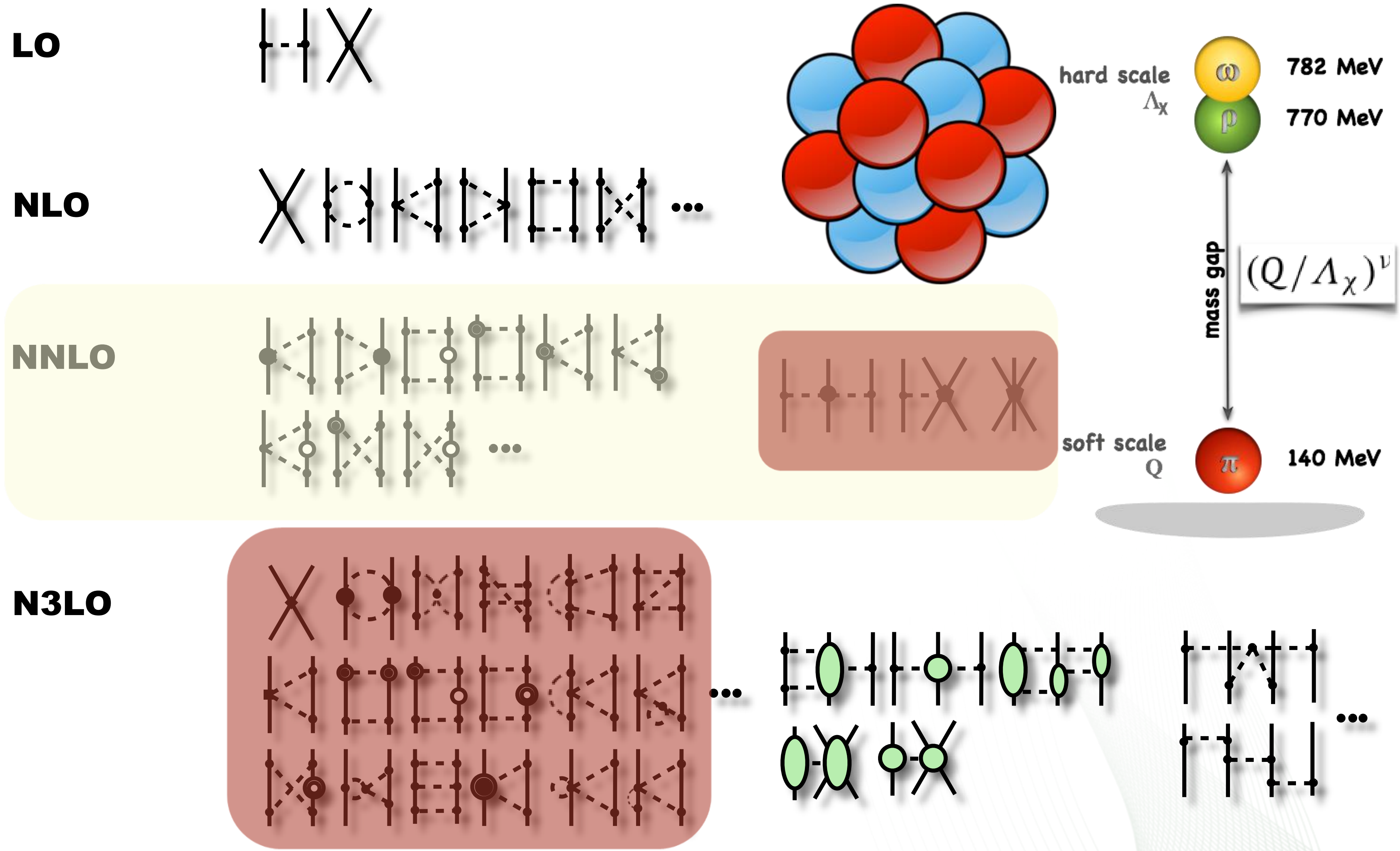


The nuclear Schrödinger equation

$$H\Psi = E\Psi$$

1. We don't know the Hamiltonian!
2. We can't solve the equation!

Chiral effective field theory (χEFT)

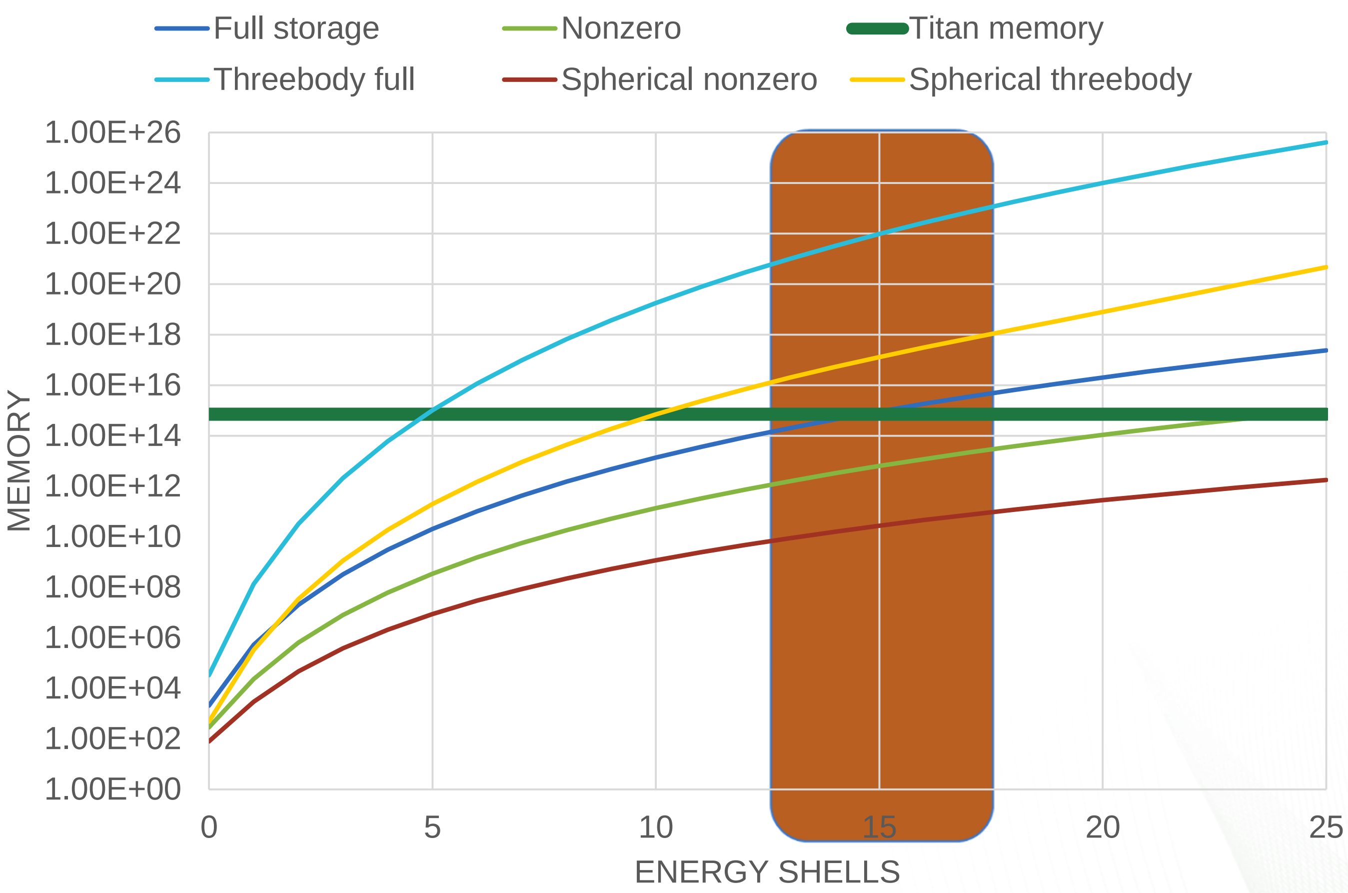


Computing the interaction

- Not possible to do “on the fly”.
- Three-nucleon forces takes weeks to transform to single particle coordinates.

The interaction elements have to be stored in memory!

Memory usage



Three nucleons forces

- Hartree-Fock with full three-nucleon force
  - Current limit: Nmax=14, E3max=18
    - ~10 TB total memory
    - Titan : 10-20% for 1 hour
    - Need larger modelspaces beyond ^{52}Ca
- Normal-ordered twobody approximation (NO2B)
  - Keep only contributions to:
    - Vacuum energy
    - Onebody operator
    - Twobody operator
- Residual three-nucleon force with $T_3^{(1)}$ (MBPT2).
  - 1 % effect (0.1 MeV per Nucleon)

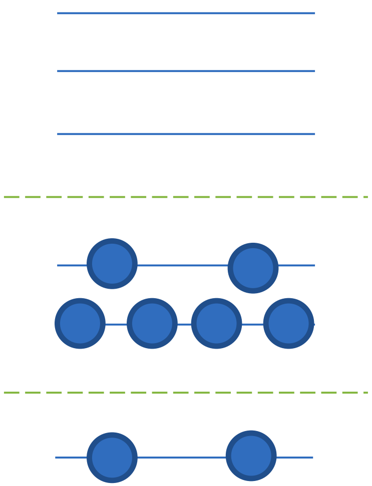
The nuclear Schrödinger equation

$$H\Psi = E\Psi$$

1. We don't know the Hamiltonian!
2. **We can't solve the equation!**

The basis

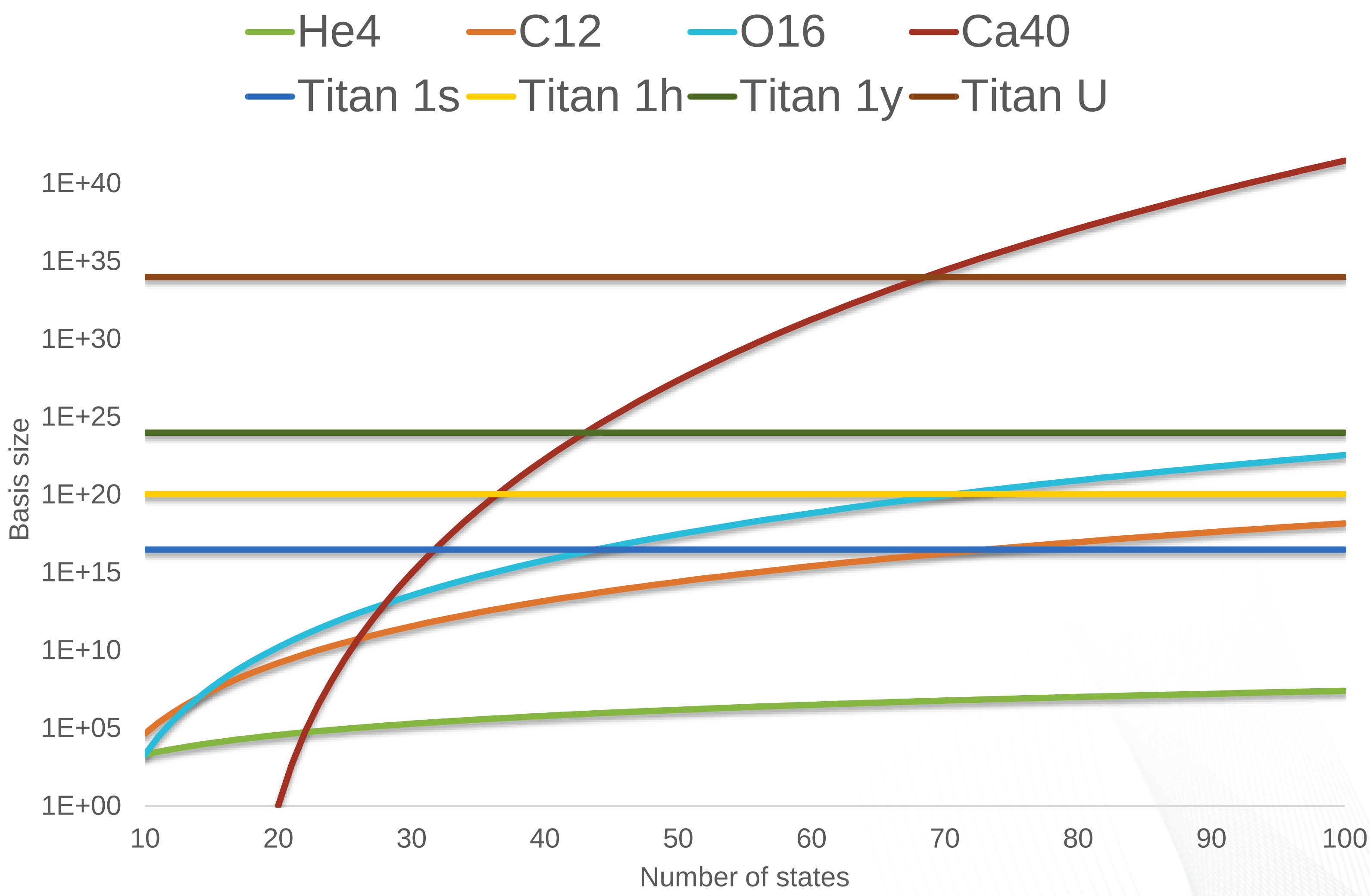
Quantum mechanics



Fermions

$$\binom{N}{A}$$

Basis size



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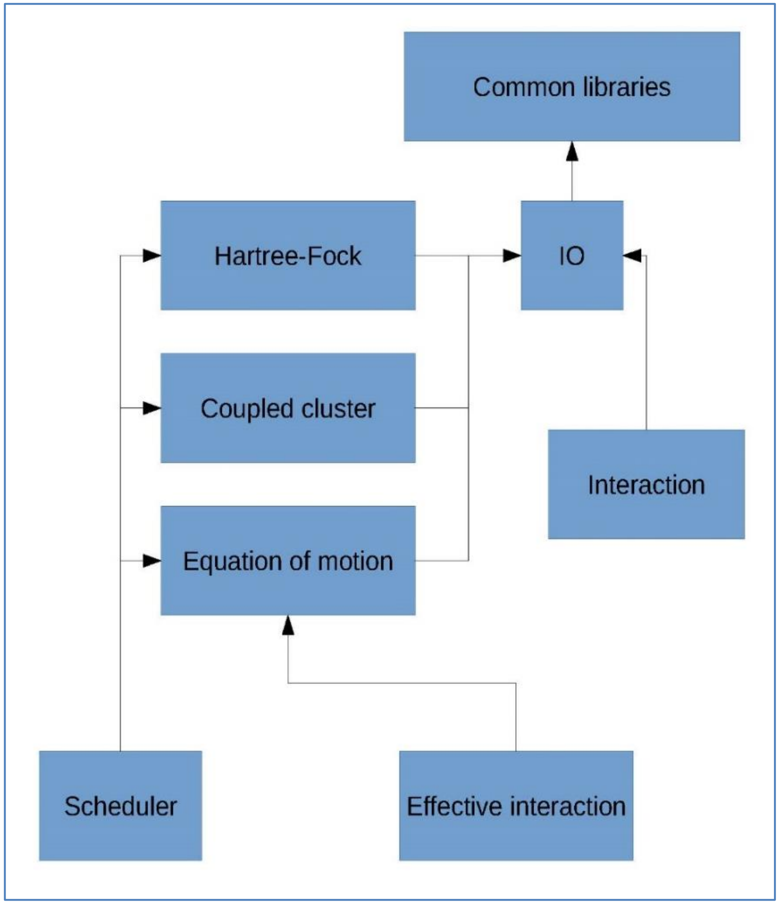
Strategy (NUCCOR)

- Large set of single-particle states
  - Extrapolate to infinity (if possible)
- Two- and three-nucleon interaction
- Treat all nucleons identically
- Find invariant subspaces
  - Isospin projection
  - Total parity
  - Total angular momentum
- Restrict basis set (2p2h, 3p3h, …)
- Reduce the number of nucleons (CCEI)
  - Frozen core
  - Effective interactions
  - Effective operators

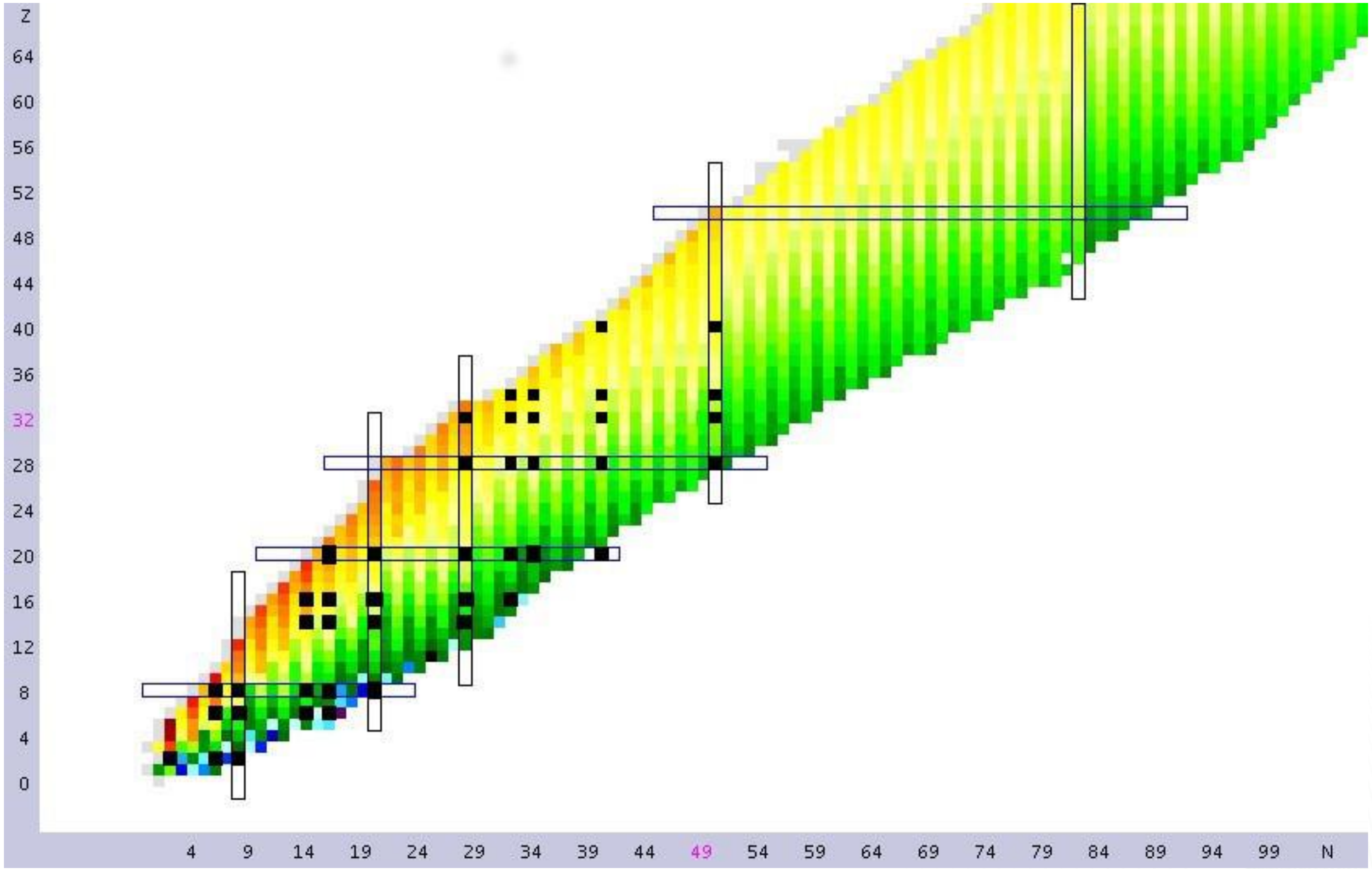
NUCCOR organization



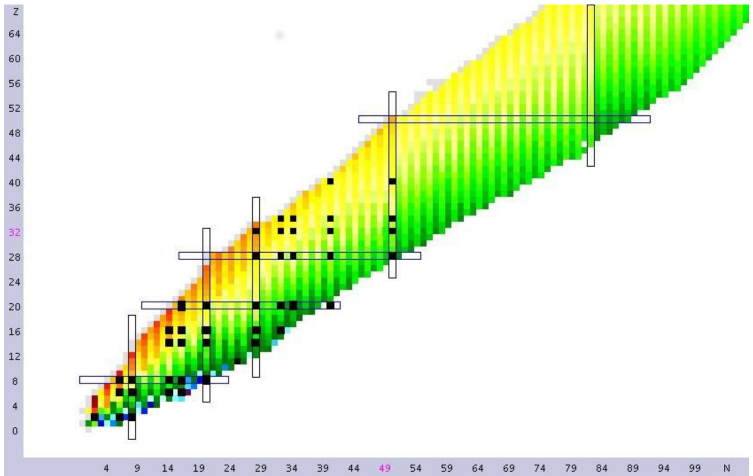
- Accepted CAAR project for CORAL
  - Will run at OLCF, ALCF and NERSC
- Runs on Titan
  - INCITE project for Nuclear Structure and Reactions
- Written in Fortran
  - MPI + OpenMP
  - 100.000 lines of code
    - F77/F95/F2003/F2008
    - Pre- and post-processing in Python
  - Stand-alone IO library (Fortran, C, & Python)
- Challenges
  - Calculating the three-nucleon interaction
  - Hartree Fock/CC with three-nucleon forces
  - Equation of motion (eigenvalue problem using Arnoldi/Non-symmetric Lanczos)

Public version available 2015/2016

NUCCOR coverage



Closed (sub-)shell nuclei

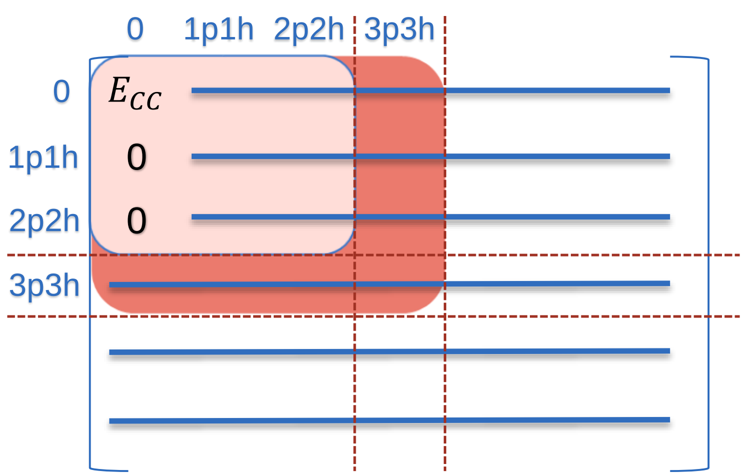


Coupled-cluster summary

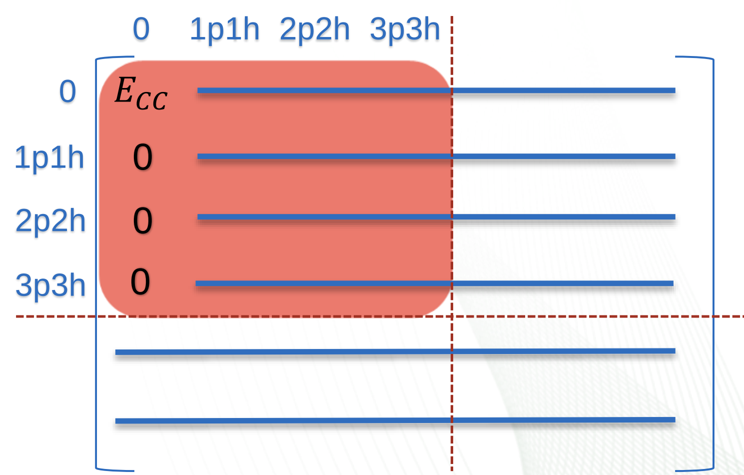
$$|\Psi\rangle = e^{T}|\Phi_0\rangle$$

$$T = T_h^p + T_{2h}^{2p} + T_{3h}^{3p} + \cdots$$

$$\overline{H} = e^{-T} H e^{T}$$

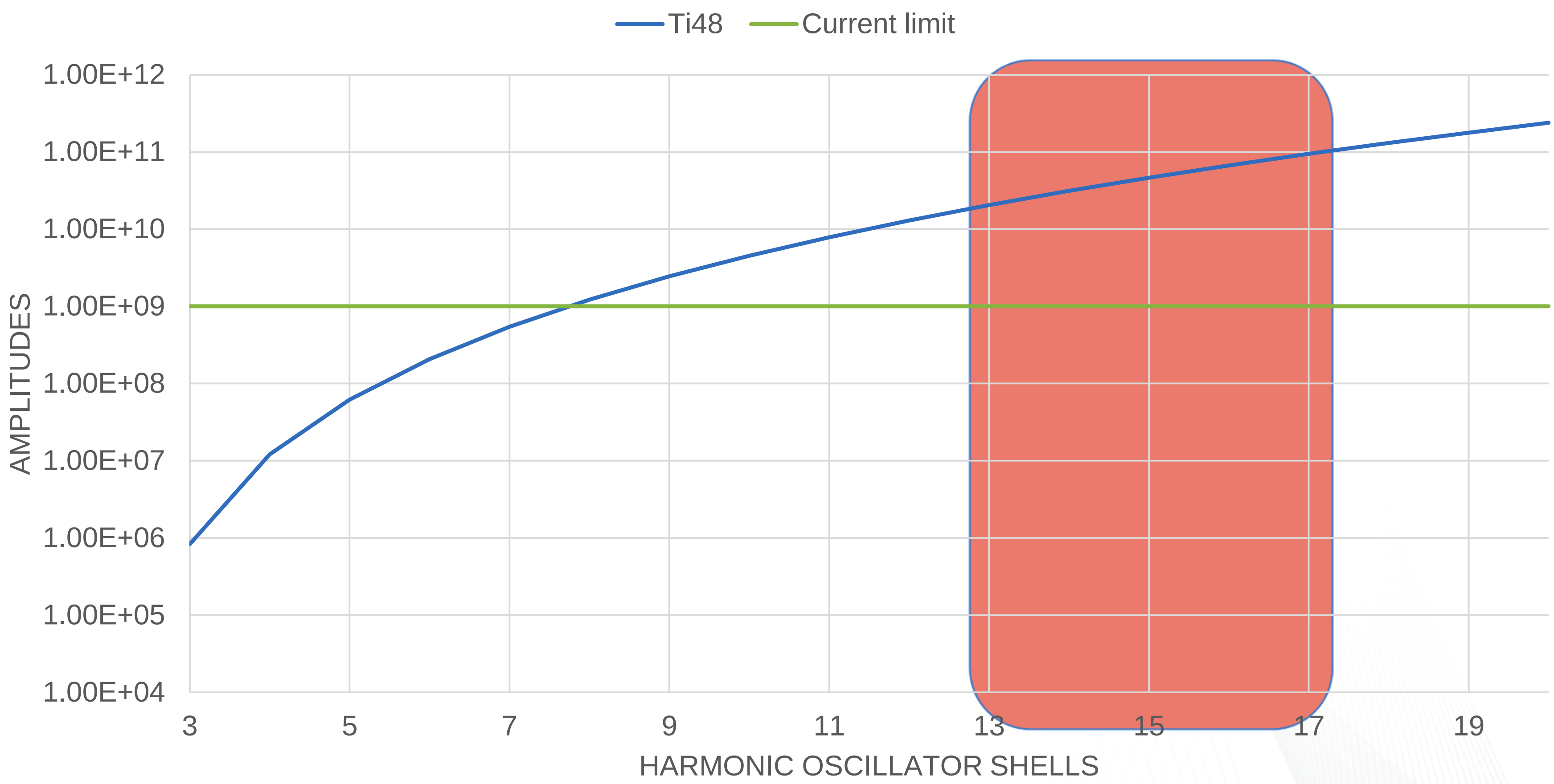


CCSD

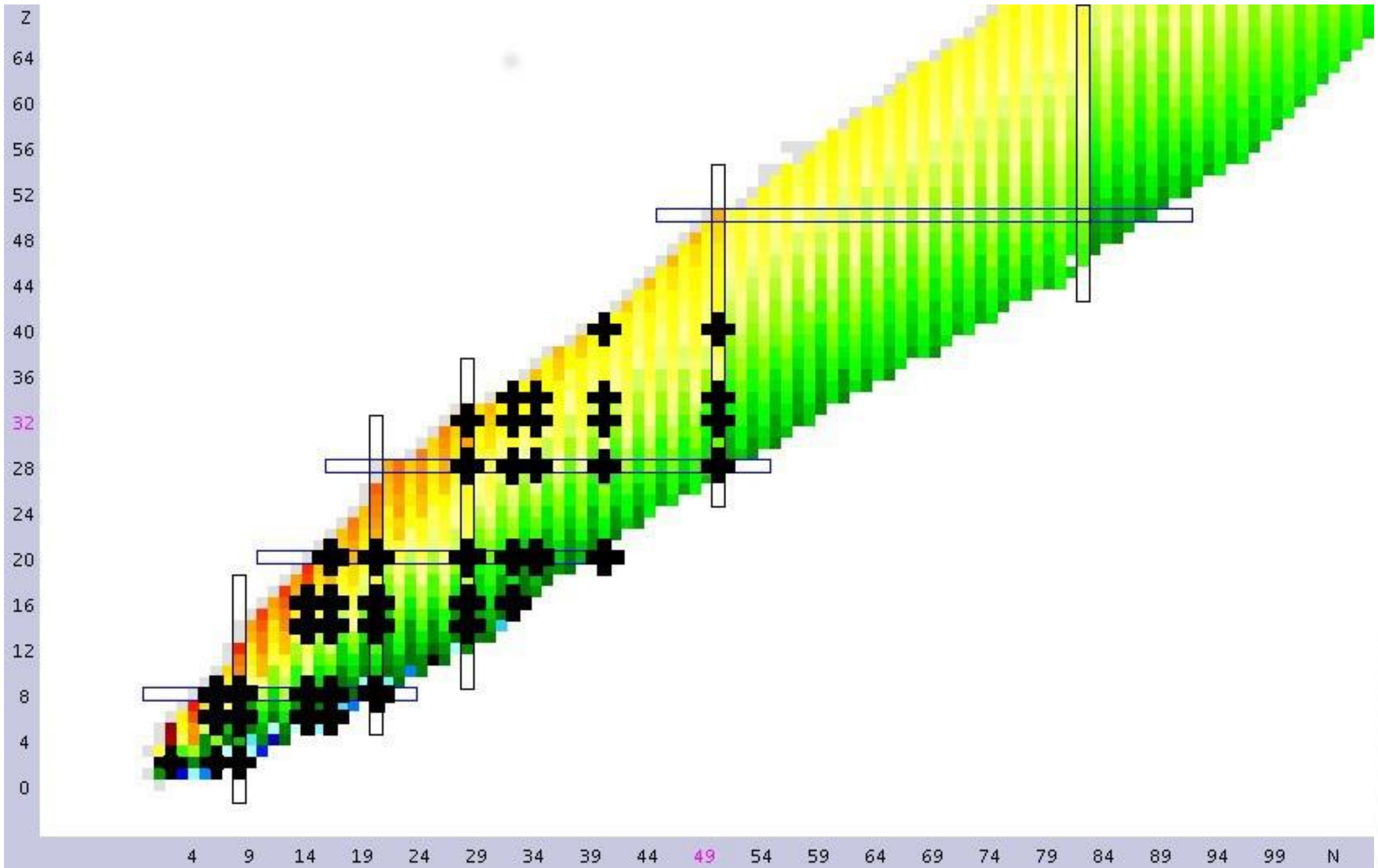


CCSDT

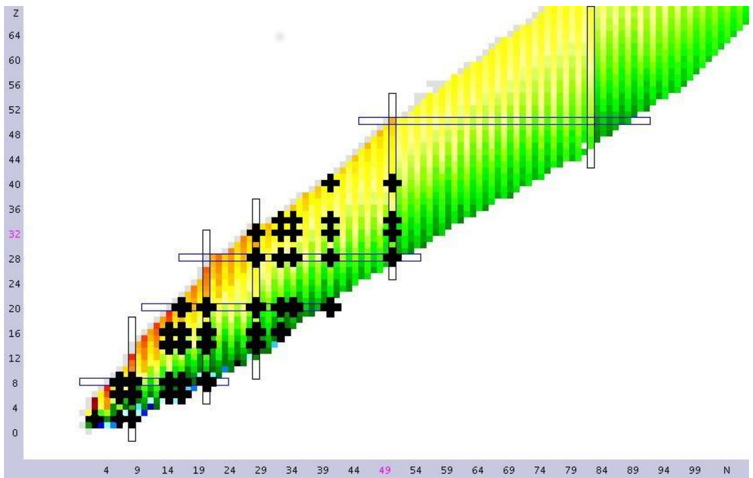
Example: ^{48}Ti



NUCCOR coverage (PA/PR)



One particle attached or removed

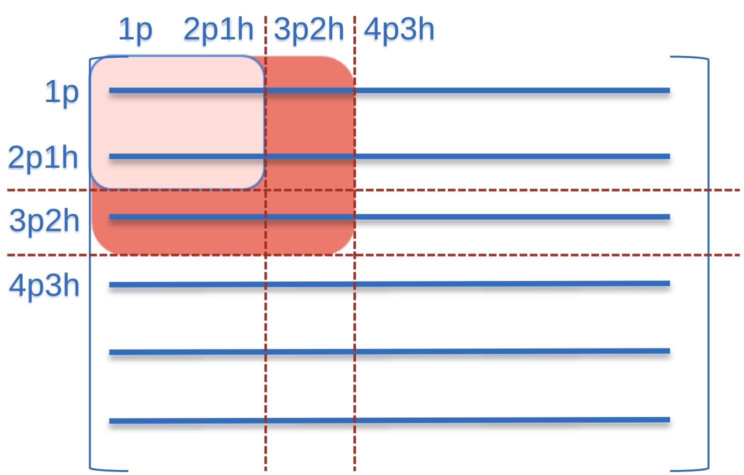


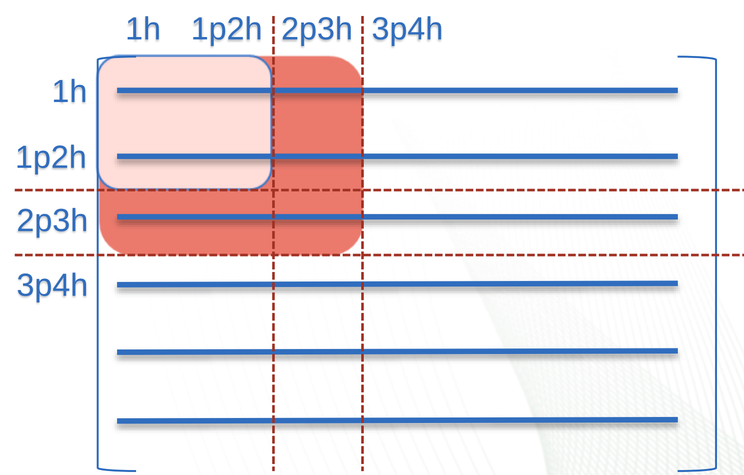
PA/PR-EOM operators

$$\overline{H} = e^{-T} H e^{T}$$

$$R^{A+1} = R^{p} + R^{2p}_{h} + R^{3p}_{2h} + R^{4p}_{3h} + \cdots$$

$$R^{A-1} = R_{h} + R^{p}_{2h} + R^{2p}_{3h} + R^{3p}_{4h} + \cdots$$





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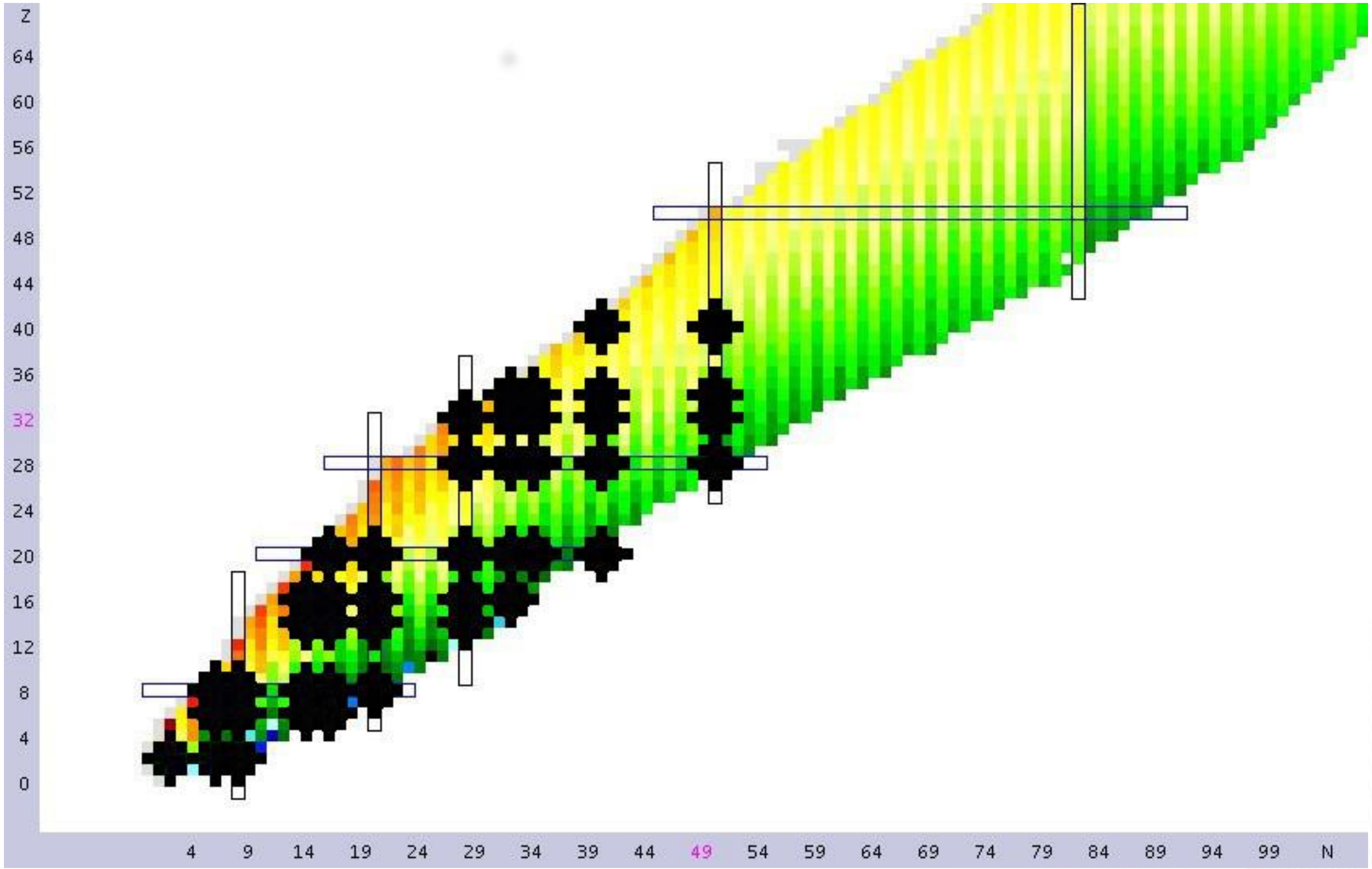
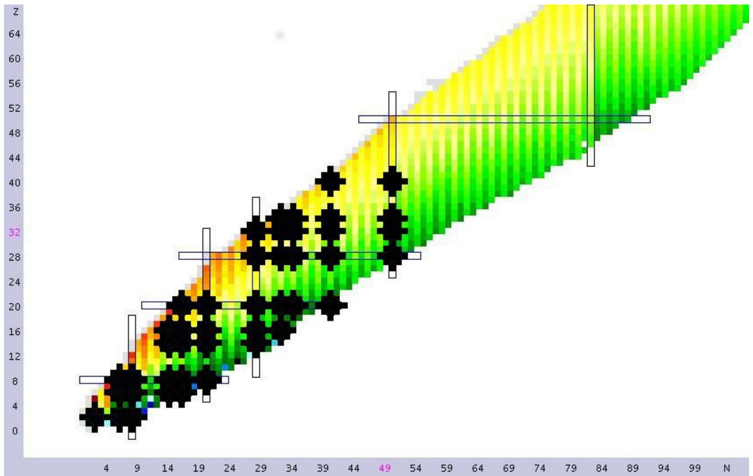
NUCCOR coverage (2PA/2PR)



Two particles attached or removed

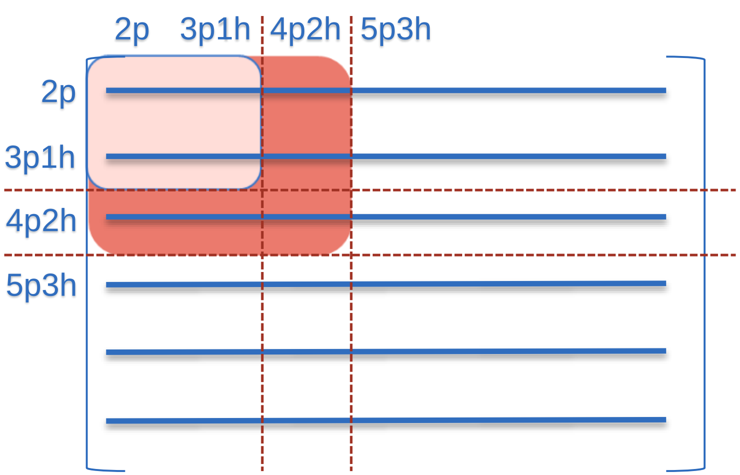


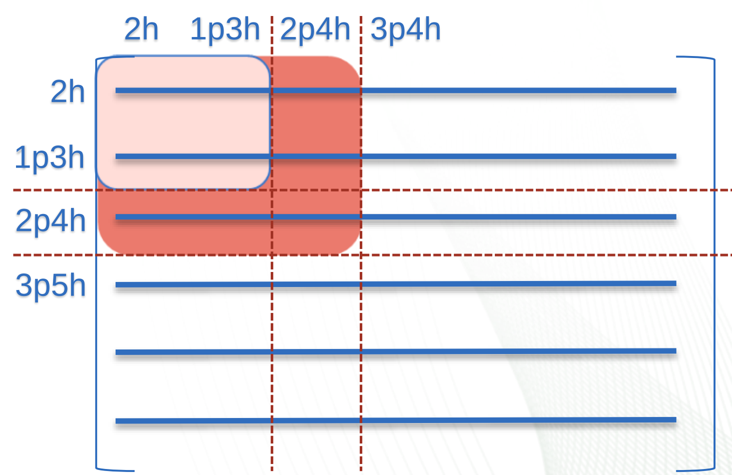
2PA/2PR-EOM operators

$$\overline{H} = e^{-T} H e^{T}$$

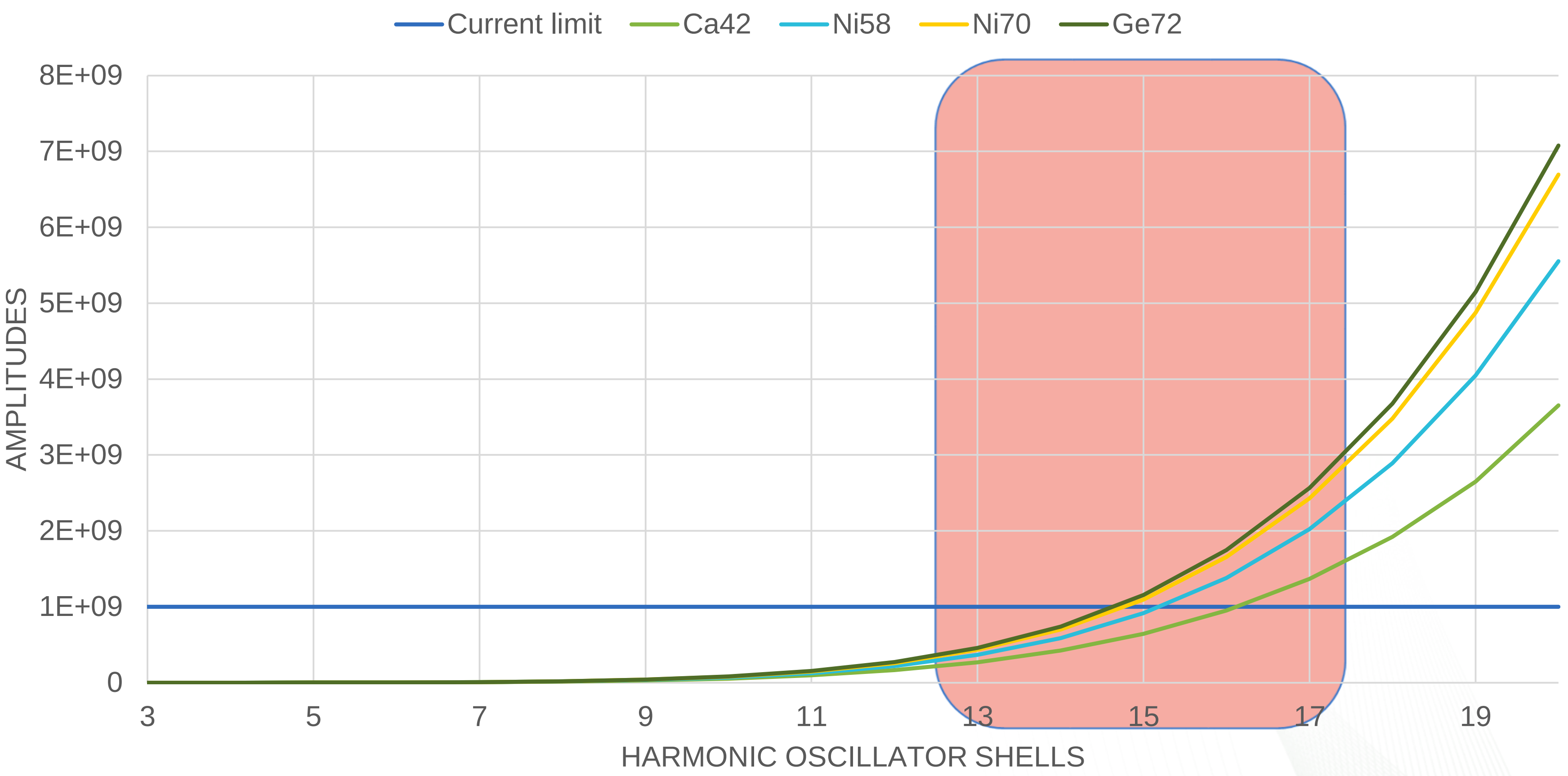
$$R^{A+2} = R^{2p} + R^{3p}_{h} + R^{4p}_{2h} + R^{5p}_{3h} + \cdots$$

$$R^{A-2} = R_{2h} + R^{p}_{3h} + R^{2p}_{4h} + R^{3p}_{5h} + \cdots$$





Example: 2PA



Current limit
Ca42
Ni58
Ni70
Ge72
AMPLITUDES
8E+09
7E+09
6E+09
5E+09
4E+09
3E+09
2E+09
1E+09
0
3
5
7
9
11
13
15
17
19
HARMONIC OSCILLATOR SHELLS

Coupled-cluster effective interaction(CCEI)

Decide on a valence space **V.**

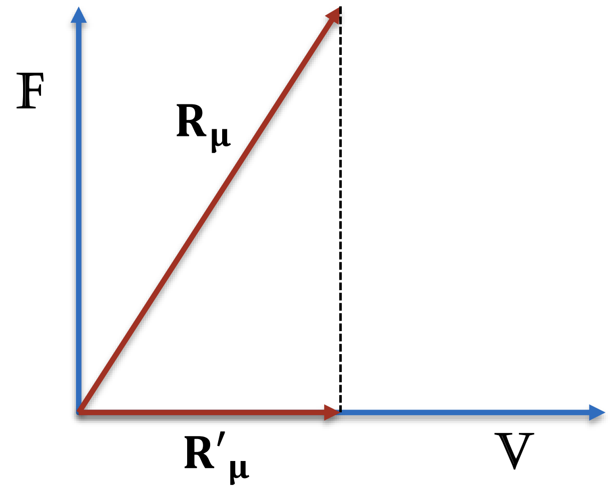
Need a twobody interaction in V that reproduce a set of chosen eigenvalues.

Find as many eigenpairs ($\mathbf{R}_{\mu}^{A+2}$,E_{μ}) in the full space, as there are twobody configurations in **V.**

Project the full eigenvectors onto **V** to find the eigenvectors of the effective Hamiltonian $\mathcal{H}$.

Construct $\mathcal{H}$ using its eigenpairs.

Final symmetric Hamiltonian after a symmetric orthogonalization step.



$$\overline{H}\mathbf{R}_{\mu}^{A+2} = E_{\mu}\mathbf{R}_{\mu}^{A+2}$$

$$\mathrm{V} = [\mathbf{R}'_1\ \mathbf{R}'_2\ \cdots \mathbf{R}'_n]$$

$$\mathcal{H} = \mathrm{V}^{-1}\mathrm{E}\mathrm{V}$$

$$\mathbf{\Theta} = \mathrm{V}^{-1}\overline{\mathbf{O}}\mathrm{V}$$

Bloch-Brandow effective interaction (Lee-Suzuki similarity transformation)

Solve for the A_c+2 problems via two-particle attached equation-of-motion coupled-cluster

$$\overline{H} R_\mu^{A_c+2} |\Phi_0\rangle = \omega_\mu R_\mu^{A_c+2} |\Phi_0\rangle$$

$$\langle \Phi_0 | L_\mu^{A_c+2} \overline{H} = \omega_\mu \langle \Phi_0 | L_\mu^{A_c+2}$$

To obtain H_{eff} we can either project the left or the right solutions onto the P-space:

$$|\psi_k^{\text{eff}}\rangle \equiv P | R^{A,A_c+2} \rangle$$

Using the right eigenvector projections we obtain CCEI:

$$\langle \alpha_P | \overline{H}_{\text{eff}}^{A,A_c+2} | \alpha_{P'} \rangle = \sum_{k=1}^{d} \langle \alpha_P | R_k^{A,A_c+2} \rangle e_k \overline{\langle \alpha_{P'} | R_k^{A,A_c+2} \rangle}$$

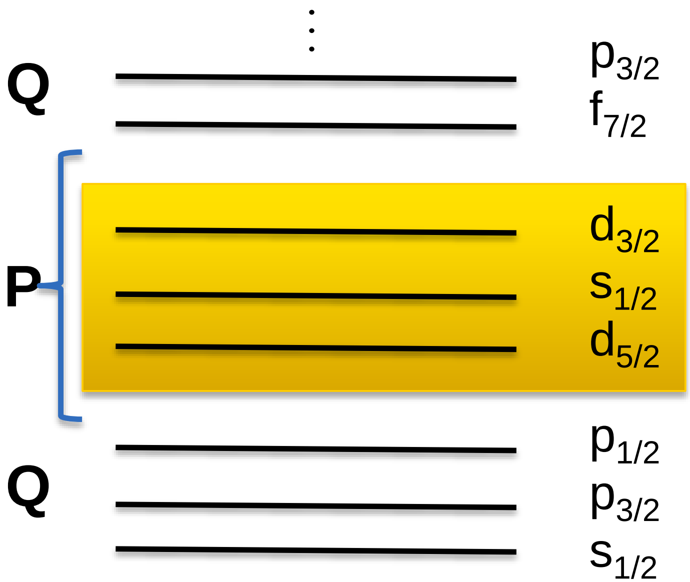
We can hermitize H_{CCEI} by using the operator S that diagonalizes H_{CCEI}

$$\left[S^\dagger S\right]^{1/2} \overline{H}_{\text{CCEI}}^{A} \left[S^\dagger S\right]^{-1/2}$$

CCEI: Application to the oxygen chain

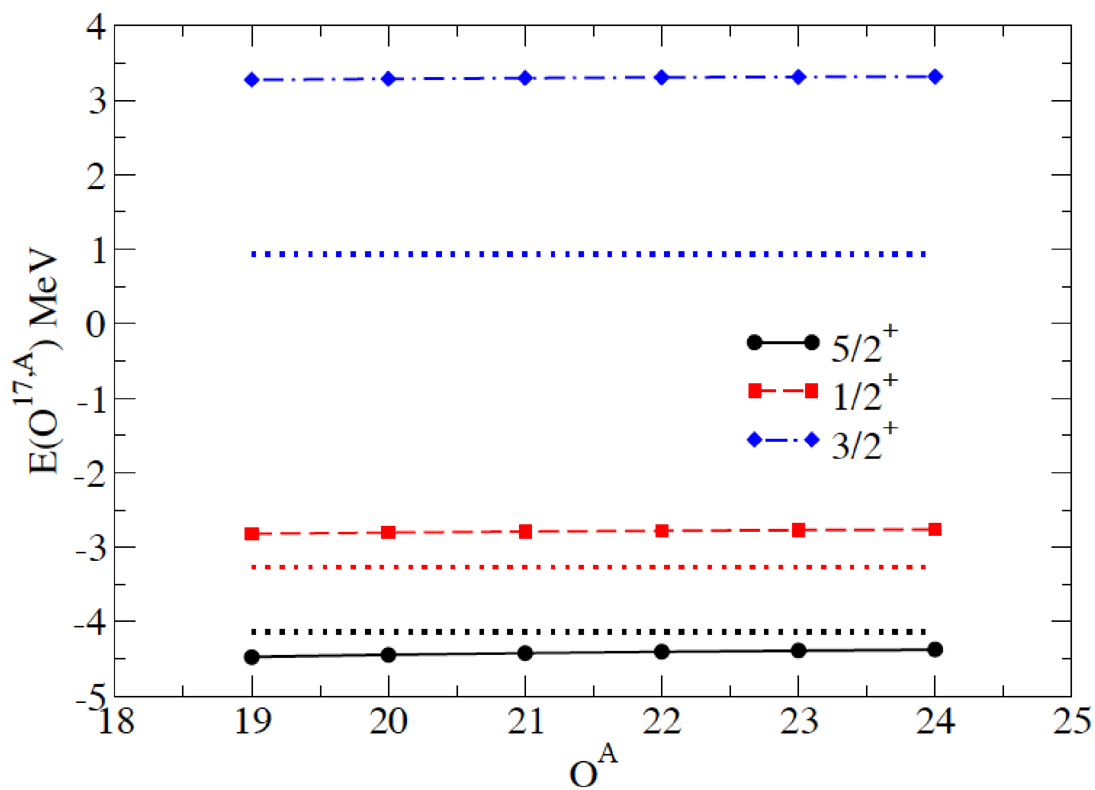
G. R. Jansen, J. Engel, G. Hagen, P. Navratil, A. Signoracci, PRL **113**, 142502 (2014).

- Start from chiral NN(N3LO$_{EM}$) + 3NF(N2LO) interactions SRG evolved to 2.0fm^{-1}
- Model space size N_{max} = E_{3max} = 12, hw = 20MeV



- Diagonalize the effective hamiltonian in the valence space.

Low-lying states in ^{17}O as a function of *A*. These energies defines the single-particle energies of H_{eff}



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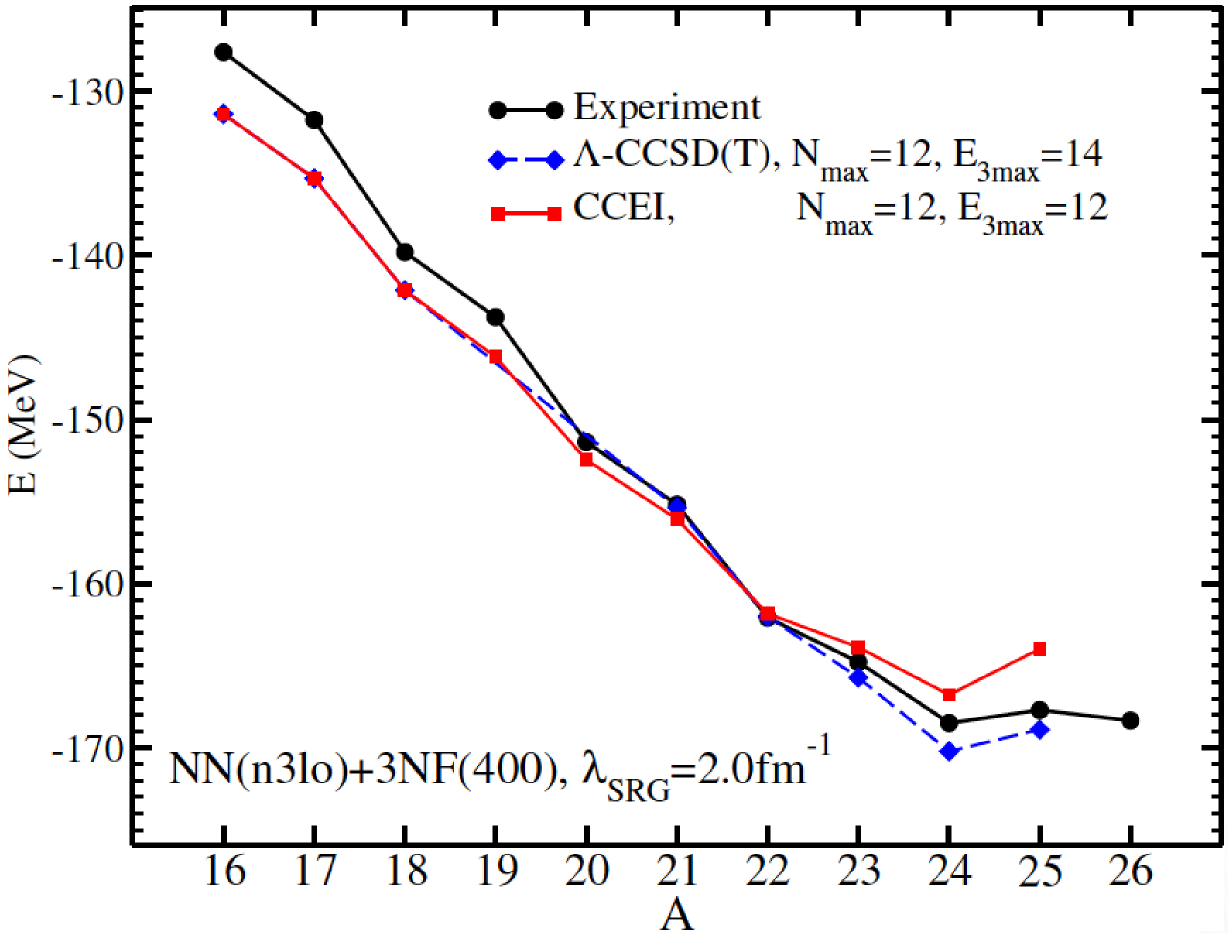

Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster.

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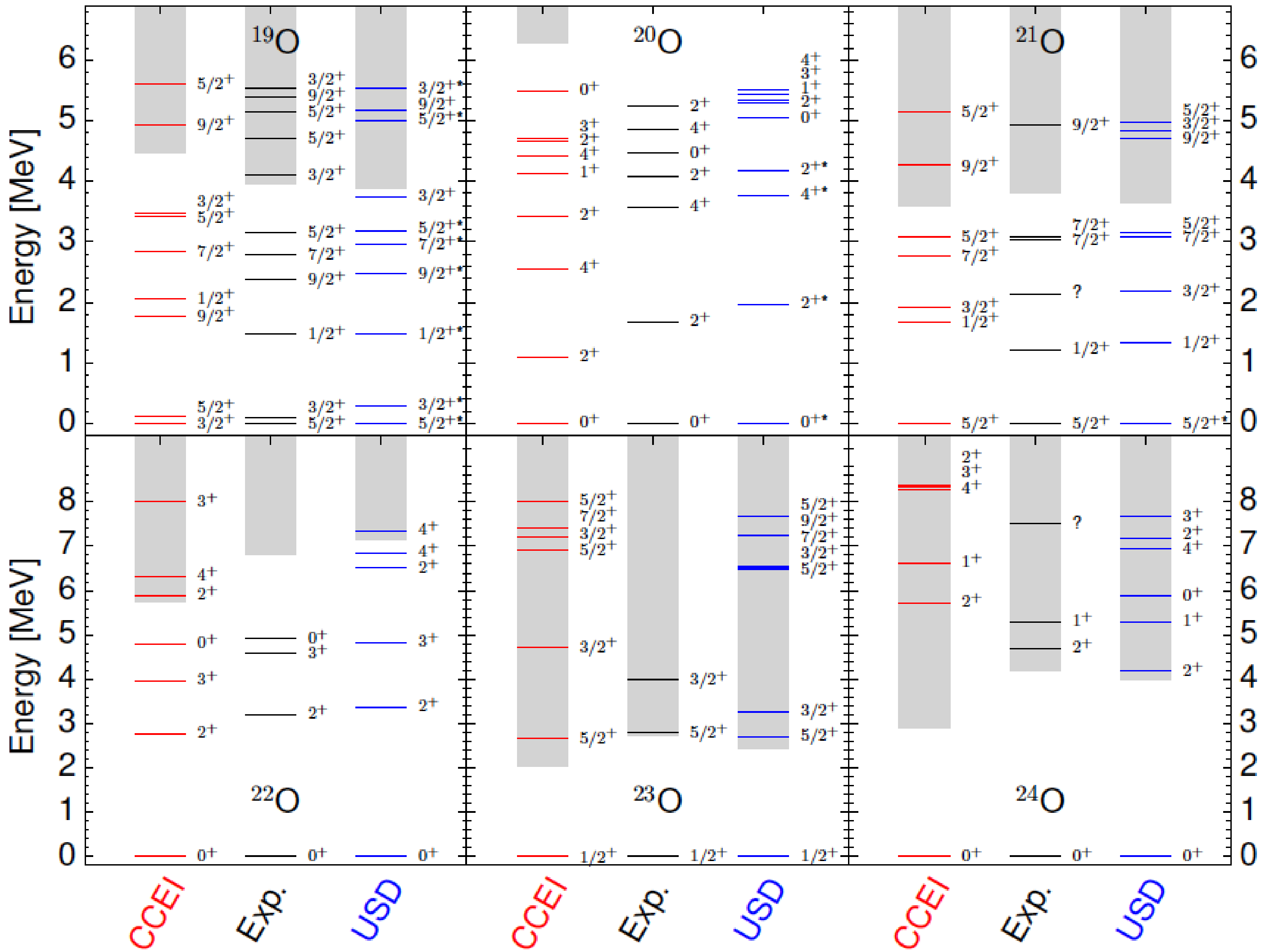
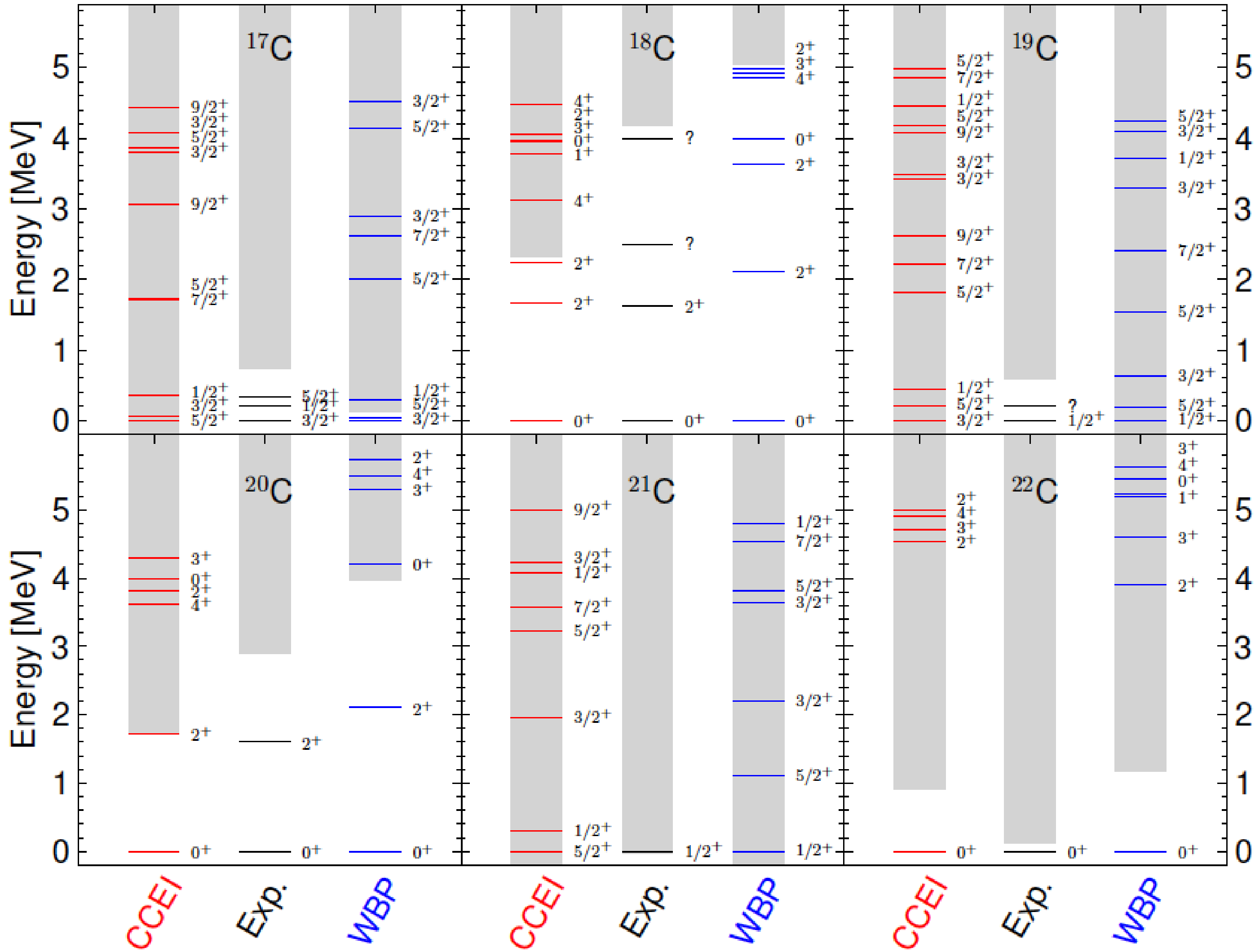
Coupled-cluster effective interactions for the shell model: Oxygen isotopes



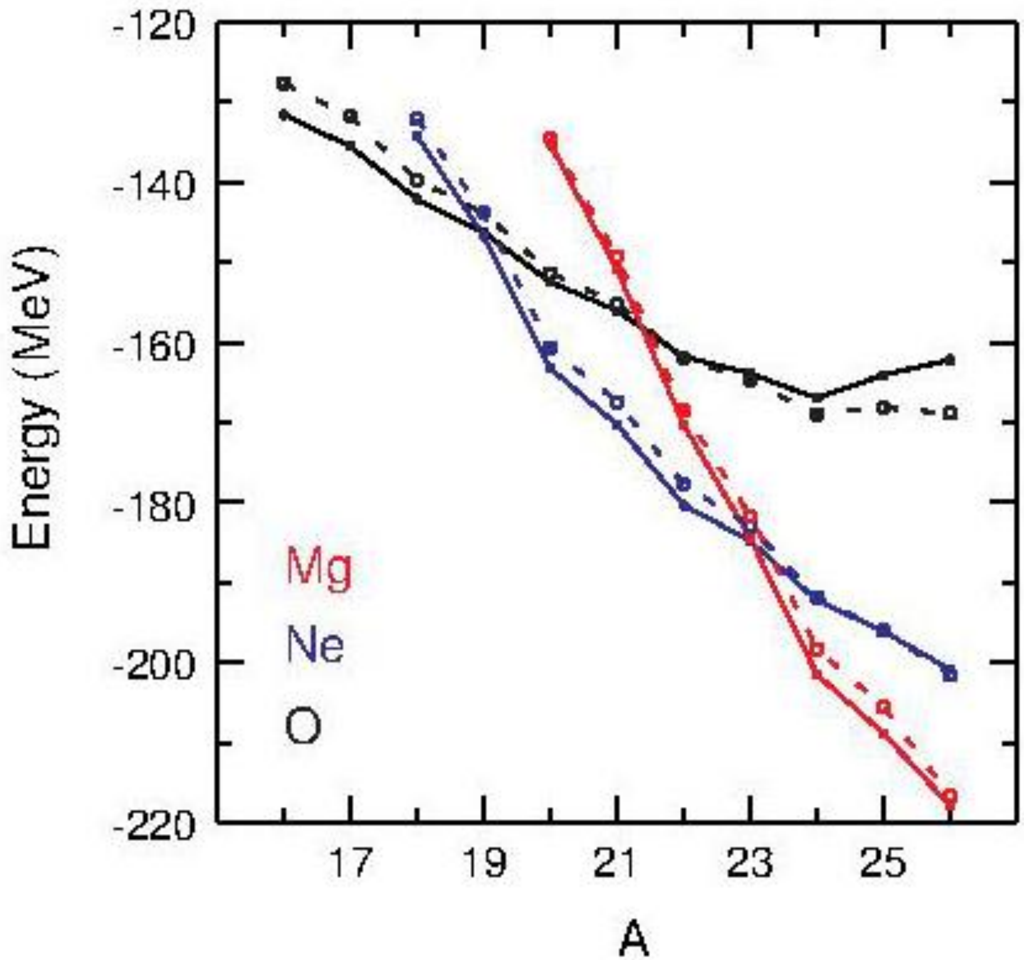
Coupled-cluster effective interactions for the shell model: Carbon isotopes



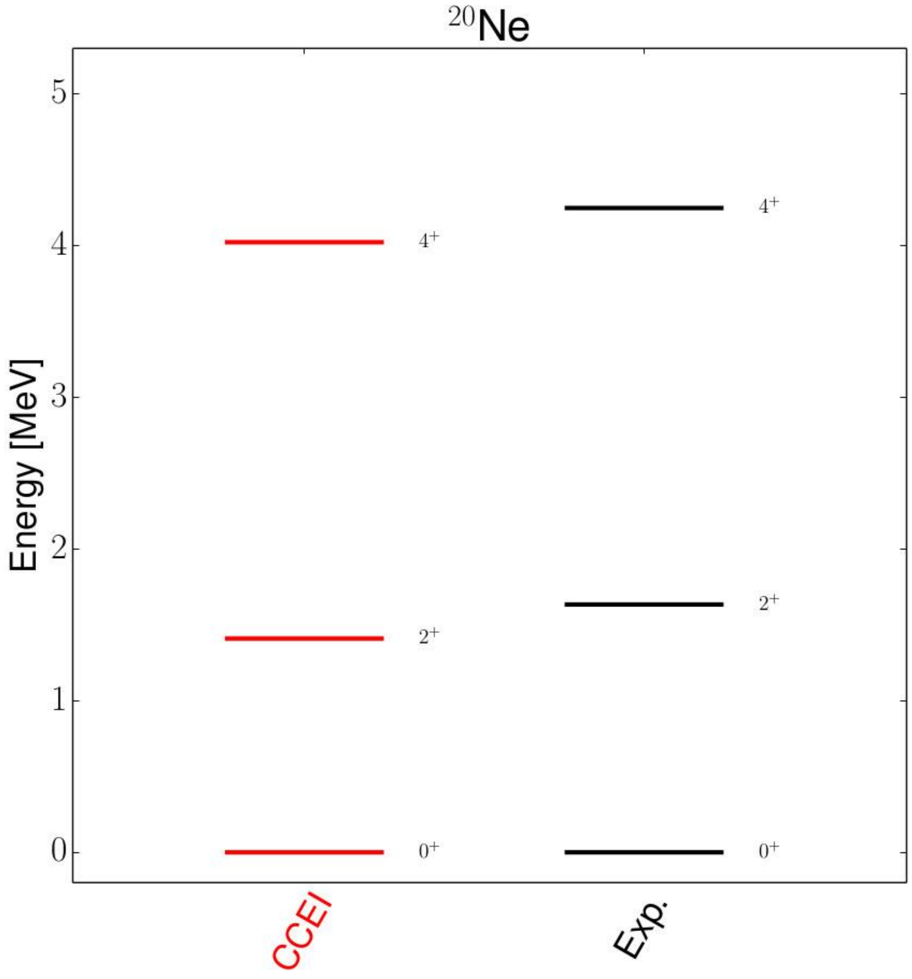
Work in progress

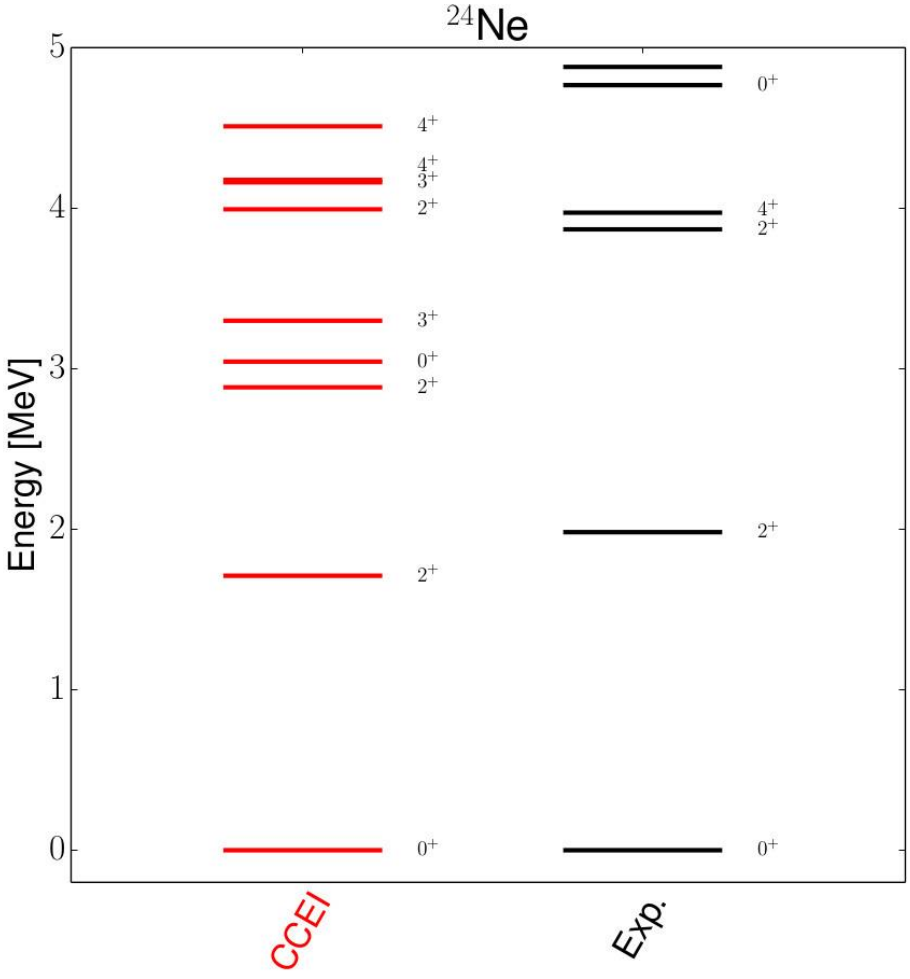
- Angelo Signoracci
- Gaute Hagen
- Petr Navratil
- Gustav R. Jansen

Binding energies



Extending CCEI to open-shell and deformed nuclei: ^{20,24}Ne and ^{23,24}Mg





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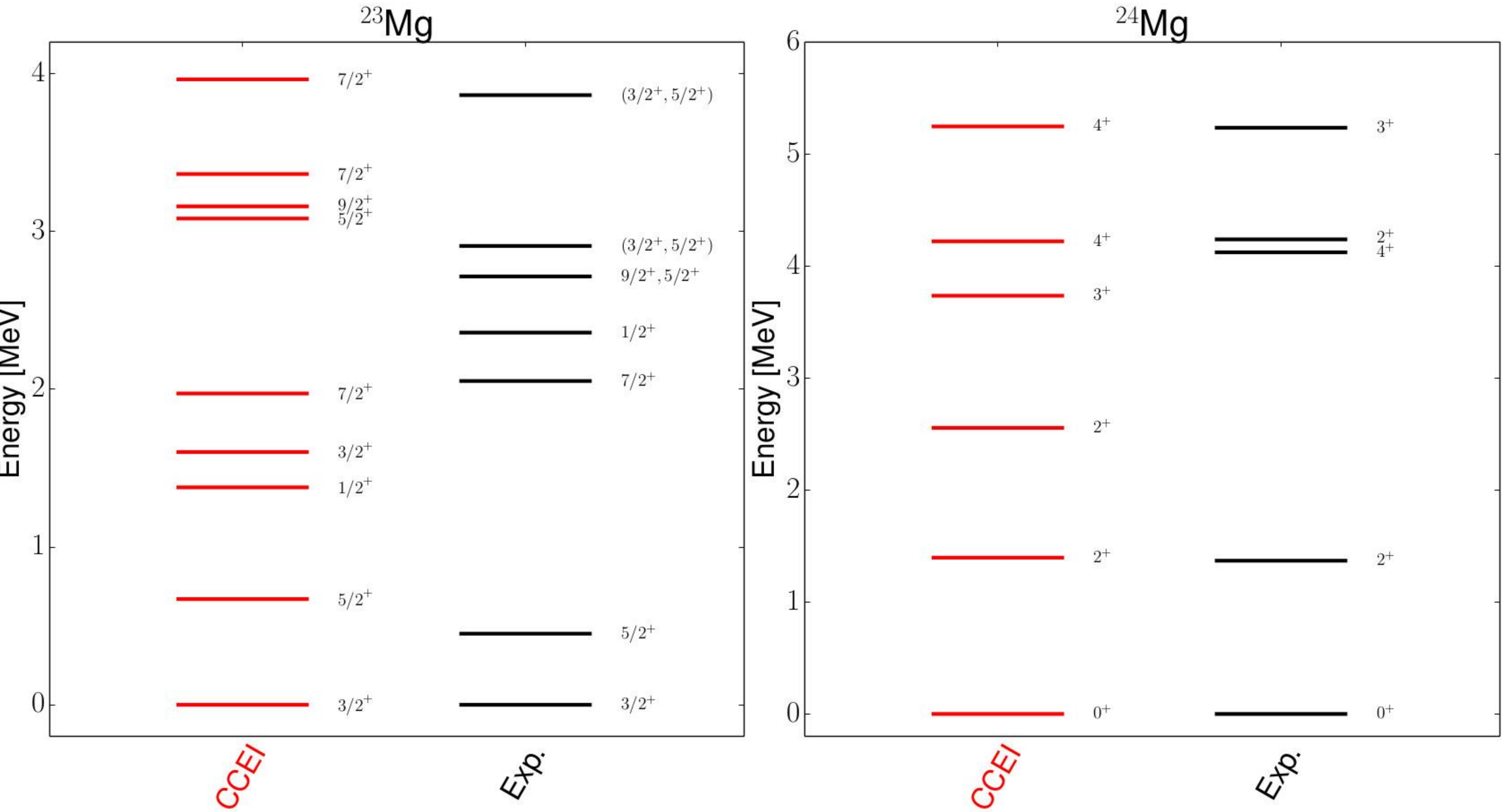
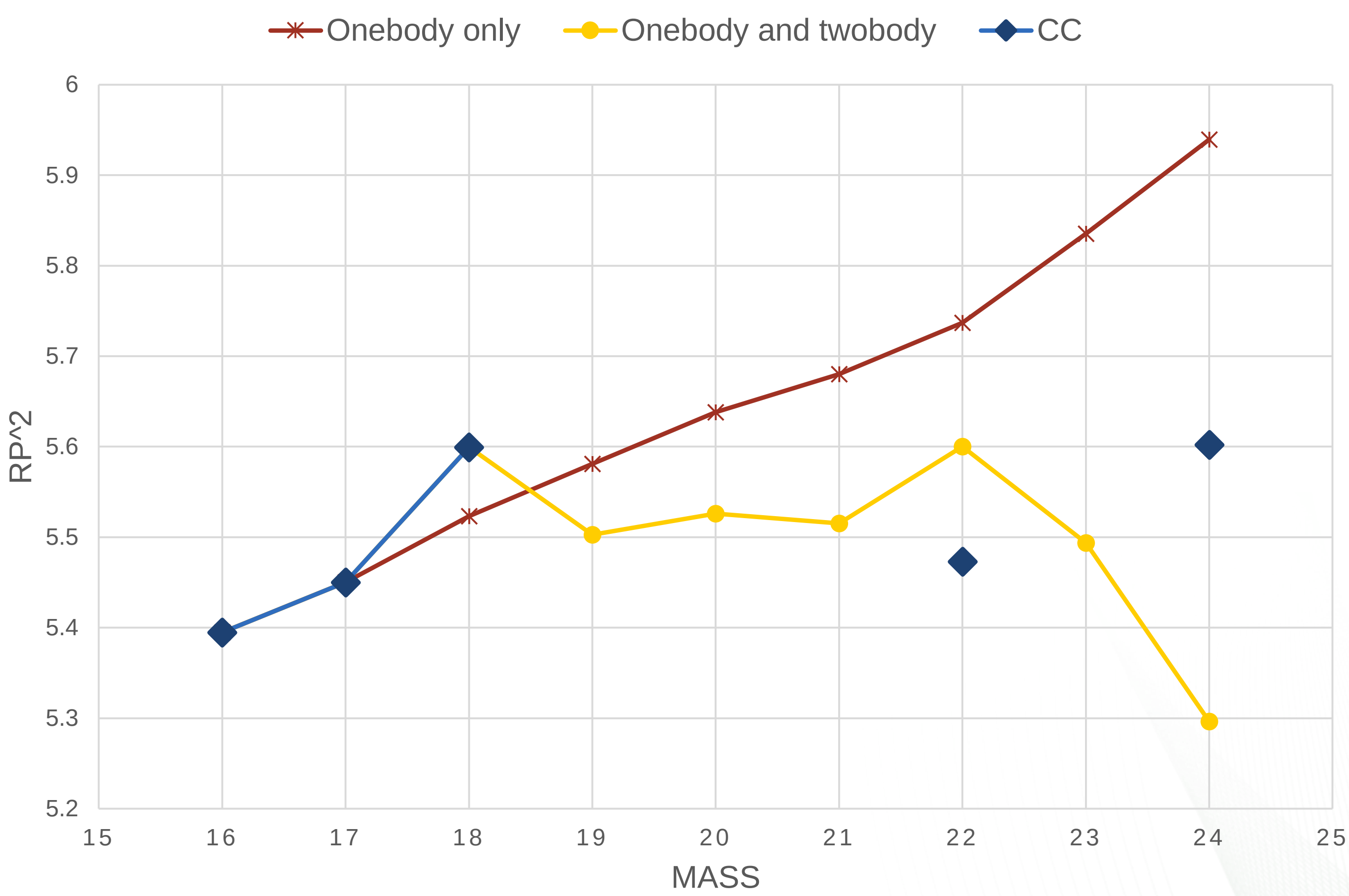


CCEI: Source of uncertainty

- Single particle energies
  - How are these calculated?
  - Need more correlations in the wavefunctions?
  - Continuum degrees of freedom.
- A+2 body wavefunctions
  - Freedom in which eigenvectors to choose.
    - Lowest energy or largest overlap with valence space.
  - Different level of convergence.
  - Center-of-mass effects.
- Valence space
  - Larger valence space?
  - Uncontrolled projection.

Effective operator: Point proton radius



Challenges

- Three-nucleon forces in HF, CC and EOM-CC.
  - Residual three-nucleon forces contribute > 1%
  - Needs to be included in CC.
- Additional correlations in EOM-CC.
  - Not possible to include the full set of amplitudes.
  - Active spaces?
- Larger modelspaces (three-nucleon force).
  - Nmax=14, E3max=18 not enough
  - Quickly saturates the available computational resources.
- Cross shell effective interactions and operators
  - Computation of A+2-body wavefunctions is the bottleneck.

Outlook

- Bigger, better, faster
  - More memory (three-nucleon forces)
  - Better algorithms and use of accelerators
  - Higher order corrections
- Uncertainty quantification
  - Theoretical error from interaction
  - Errors from optimization and extrapolations
  - Theoretical error from manybody calculations
- (Grand) challenge problems
  - Neutrinoless double beta-decay
  - Limits of stability
  - Open-shell nuclei

Questions?

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